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# Coherent *X*-ray scattering data for plastics

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***Abstract***

*Coherent x-ray scattering data including molecular interference effects are obtained for plastics. To determine the effect of molecular interference, the molecular form factors are calculated. The theoretical results of molecular form factors are compared with experimental values in literature. The molecular form factors varies importantly for low momentum transfer values. As a result of this, for very low photon energies, a significant change in the coherent scattering cross sections is observed. The interference effects are the main cause of form factor and coherent scattering coefficient differences. The results obtained in this study will provide remarkable data for use by others to model photon transport problems.*

***Keywords****: Plastics, coherent x-ray scattering, interference effects.*

# Plastikler için Coherent *X*-ışını saçılma verileri

***Özet***

*Girişim etkilerinin dahil edildiği koherent x-ışını saçılma verileri plastikler için elde edilmiştir. Moleküler girişimin etkisini belirlemek için, moleküler form faktörler hesaplanmıştır. Moleküler form faktörlerin teorik sonuçları literatürdeki deneysel değerler ile karşılaştırılmıştır. Moleküler form faktörler düşük momentum transfer değerleri için önemli bir biçimde değişmektedir. Bunun sonucu olarak, çok düşük foton enerjileri için, koherent saçılma tesir kesitlerinde önemli bir değişim gözlenmektedir. Girişim etkileri, moleküler form faktör ve coherent saçılma tesir kesiti farklılıklarının ana sebebidir. Bu çalışmada elde edilen sonuçlar, foton transfer problemlerini modelleyenler tarafından kullanılması için kayda değer veri temin edecektir.*

***Anahtar kelimeler****: Plastikler, koherent x-ışını saçılma, girişim etkileri.*

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## 1. Introduction

Coherent scatter imaging is finding increasing use in industrial and security applications, where directly identifying the material composition has become a priority [1]. The determination of significant variation between the structural properties of different molecules and complex structures is available by using coherent scattering [1]. In the diagnostic *x*-ray energy range, there are interference effects due to the coherence of elastic scattered photons, mainly at small-angles, which causes a unique scattering signature, characteristic for each material [2]. The simulation needed to be modified to more accurately model the coherent scattering in molecules and complex structures including the interference between photons scattering from different atoms [3-4]. The interference effects are well known in the field of crystallography. In an amorphous solid, the arrangement of the molecules is not completely featureless [5]. There is still a weak ordering. Therefore, interference is also possible for coherent *x*-ray scattering from amorphous materials [5].

In this study, the x-ray coherent scattering where interference effects are taken into account is studied for plastics (polyethylene, polystyrene, polycarbonate, and nylon). The theoretical molecular form factor (FF) was carried out in the presence of concentrations of elements making up the plastic. The theoretical FF in this study is compared with the experimental FF of King et al. [6]. The molecular coherent scattering coefficients computed differently from the literature including molecular interference effects will offer more accurate information. It is expected that the results obtained in this study will provide contribute an important to the literature.

## 2. Method

### *2.1. The molecular form factors*

The form factor approximation is used to predict the x-ray coherent scattering coefficients. The experimental form factors are in better accommodation with the modified relativistic form factor (MFF) approximation [7]. The MFF approach is better than other approaches, as indicated by some researchers [7, 8-17].

For most composite materials, the molecular form factor data are calculated using the independent atomic model (IAM) or the sum rule,

$$\frac{F_m^2(x)}{W} = \sum_i \frac{w_i}{M_i} F_i^{\,2}(x, Z_i) \qquad (1)$$

where $w_i$, $M_i$, $Z_i$ and $F_i(x,Z_i)$ are the mass fraction, the atomic mass, the atomic number and the atomic FF of element *i*, respectively. *W* is the molecular weight. The $F_m(x)$ is the molecular FF as function of the momentum transfer variable $x=\lambda^{-1}\sin(\theta/2)$. The theoretical FF do not account the interference between photons scattering from different atoms but only account for the interference scattering from electrons in the same atom. Therefore, the experimental FF is used at low values of momentum transfer. The sum rule can be applied at large momentum transfer values. Because there is the asymptotic convergence between the experimental and theoretical form factors. This situation is reported by researchers [18-21].

### *2.2. The x-ray coherent scattering cross section*

The x-ray coherent scattering cross section is computerized by using the Thomson formula [22] weighted by the $F^{\,2}{}_m(x)$ over all scatter angles per molecule as

$$\sigma_{mol} = \int_{\theta=0}^{\theta=\pi} d\sigma^{T}(\theta)\left[F_m(x)\right]^2 \tag{2}$$

## 3. Result and discussion

The theoretical molecular form factor data are calculated with the MFF approximation using Eq. (1). The theoretical data in this study are shown in figure 1 together with experimental data [6]. Theoretical data provides an approximation in the region of $x \geq 10$ nm$^{-1}$ where there is no experimental data. As can be seen in figure 1, the differences between the experimental and theoretical data are observed for values of $x \leq 1.5$ nm$^{-1}$ as a result of the molecular interference effects. The experimental data shows a strong increase in the region ($x \leq 1.5$ nm$^{-1}$) where interference effects are big and the angular distribution peak at a certain angle. This angle depends on the photon energy, type and structure of plastic.

The molecular x-ray coherent scattering coefficients are calculated by using both experimental form factor which covers values of $x \leq 9.25$ nm$^{-1}$ and theoretical form factor which covers values of $10 \leq x \leq 10^3$ nm$^{-1}$. Also, the molecular coherent scattering coefficients are calculated without the inclusion of the interference effects by using only theoretical form factor which covers values of $0 \leq x \leq 10^3$ nm$^{-1}$. The molecular interference effects in x-ray coherent scattering are shown in figure 2 for each plastic material.

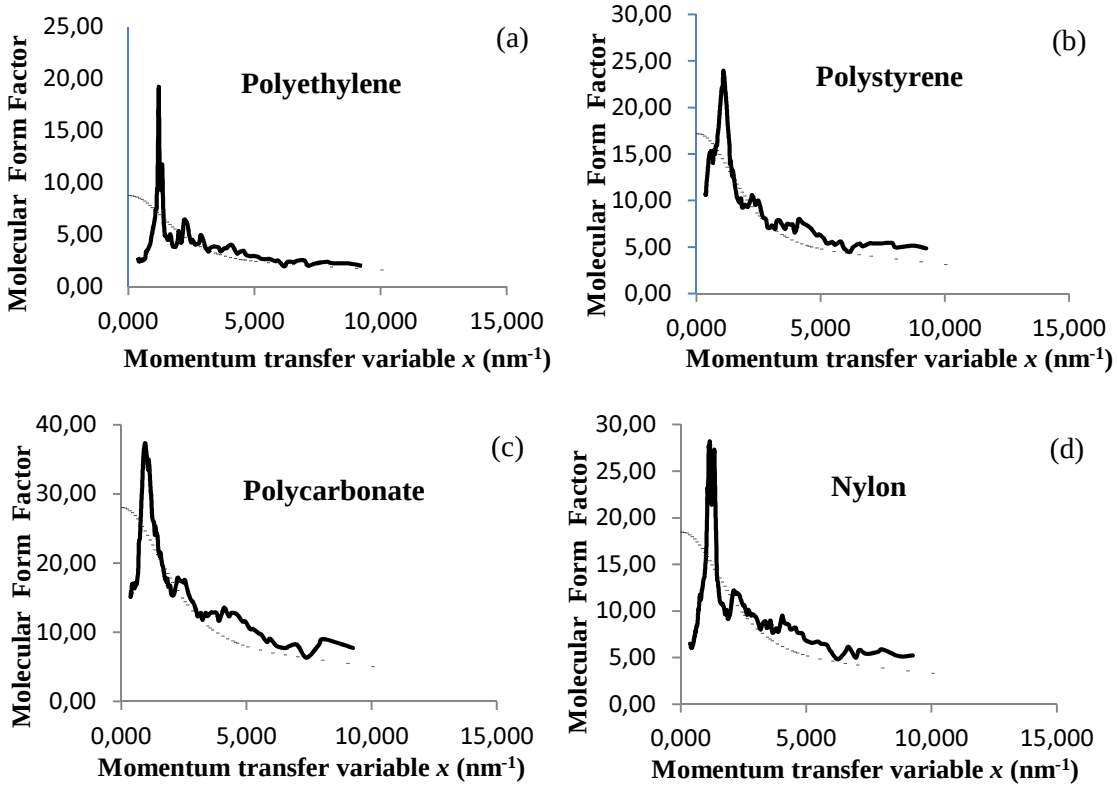


Figure 1. Comparison between experimental form factor of King et al [6] (straight line) and theoretical form factor in this study (dotted) for (a) polyethylene, (b) polystyrene, (c) polycarbonate, (d) Nylon.

As can be seen in figure 2, a significant reduction in x-ray coherent scattering coefficients was observed due to molecular interference effects for very low photon energies (~ up to 5 keV). For very low photon energies, the integration in coherent scattering cross section calculations covers small values of momentum transfer, and it causes a significant change.

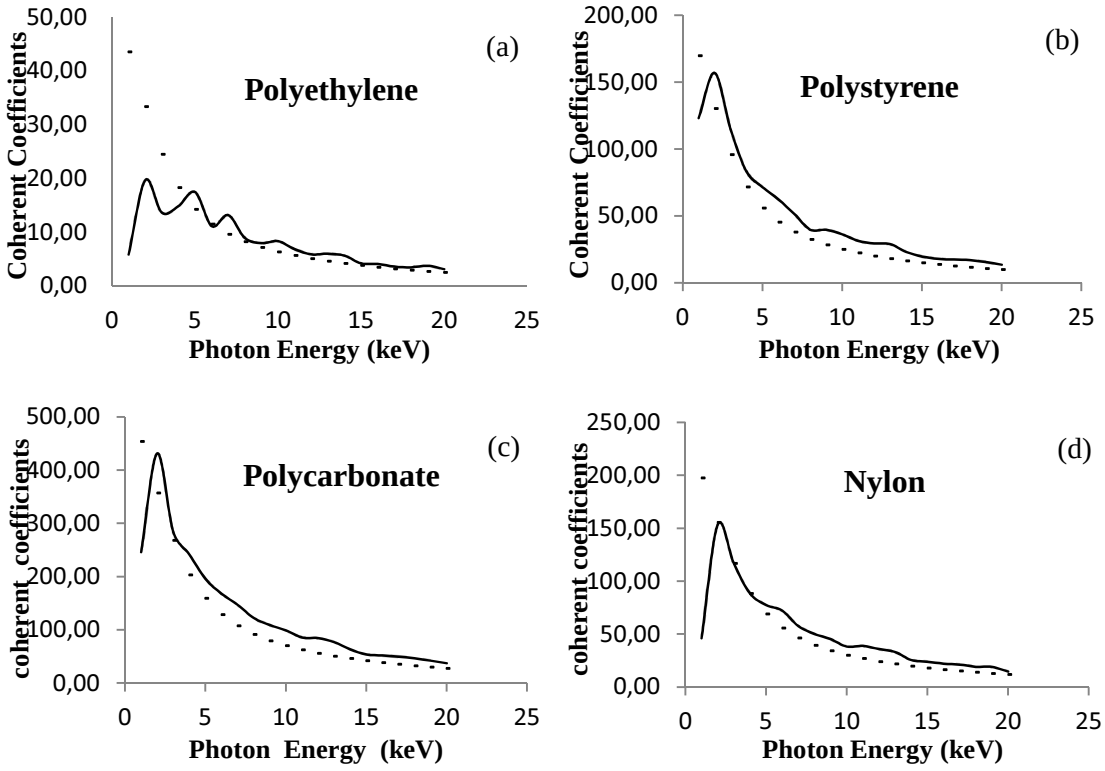


Figure 2. The molecular total coherent scattering cross sections computed with the inclusion of the molecular interference effects (straight line) and without the inclusion of the molecular interference effects (dotted) for (a) polyethylene, (b) polystyrene, (c) polycarbonate, (d) Nylon.

## 3. Conclusion

The theoretical and experimental FF are close to each other for values of $x > 1.5$ nm$^{-1}$. The differences for values of $x \leq 1.5$ nm$^{-1}$ are a result of the molecular interference effects. For the photon energies greater than 12 keV, the integration in the coherent scattering coefficient calculations extends to values of $x \geq 10$ nm$^{-1}$ and so it uses both experimental FF and theoretical FF results. Therefore, it is important that the theoretical FF is compatible with the experimental FF. For very low photon energies, it is observed that the coherent scattering data included the molecular interference effects are smaller than the coefficients calculated without molecular interference effects.

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